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Toward Fast Multipole Methods on a Lattice

ABSTRACT

We discuss the concept and implementation of fast multipole algorithms on a regular structured grid. In doing so, the discrte analogue of the continuous fundamental solution is evaluated numerically.

Toward Fast Multipole Methods on a Lattice

Lijun Jiang and Igor Tsukerman*

August 15, 2012

1 Introduction

Many applications call for a rapid evaluation of discrete convolutions of the form

$$(f * g)(\mathbf{n}) \equiv \sum_{\mathbf{k}\in\mathbb{Z}^n} f(\mathbf{k})g(\mathbf{n}-\mathbf{k}) = \sum_{\mathbf{k}\in\mathbb{Z}^n} f(\mathbf{n}-\mathbf{k})g(\mathbf{k}) \tag{1}$$

where f and g are real or complex functions on a regular lattice $\mathbb{Z}^n$. We shall be dealing primarily with the most interesting and challenging 3D case ($n = 3$).

Applications where convolutions (1) arise include (a) digital signal/image processing/ filtering by time-invariant (translation-invariant) systems and (b) finite difference analysis of boundary value problems. In the latter category, two related methodologies are particularly noteworthy. The first one, put forward and thoroughly studied by Ryaben'kii, Tsynkov and others [1, 2], is known as the method of difference potentials and can be viewed as a discrete analog of the Calderon projection operators. The second one, boundary algebraic equations (BAE), is at least 50 years old (Saltzer [16]) and is a discrete analog of first- or second-order Fredholm boundary integral equations for potential problems (Martinsson & Rodin [15]).

The primary objective of this work is to develop a Fast Multipole Method on a Lattice (FMML) for computing convolutions (1). The "source nodes" where f is nonzero are assumed to be confined to a finite box containing a fragment of the lattice; this box is recursively subdivided into a nested sequence of smaller boxes that form a tree structure (quadtree in 2D, as each box gets subdivided into four children.) In contrast, g does not have to have a bounded support; in boundary value problems, it will represent discrete Green's function.

The general principles of FMML are the same as in the well-known continuous case [3]: "far-field" contributions to the potential due to remote sources are computed via a multipole expansion, while the near field is computed directly. The multipole moments are computed in the course of the upward pass over the hierarchical structure of boxes. Then these multipole moments get converted into local field expansions in the course of the downward pass from the root box to the finest level.

The ingredients of this computational procedure are worked out below and include (i) the multipole expansion; (ii) far-field-to-far-field translation (needed in the upward pass); (iii) far-field-to-local-field and local-to-local-field translation formulas (needed for the downward pass).

A remarkable feature of the resultant algorithm is its universality: it can be applied to any given convolution kernel g (discrete Green's function in applications to boundary value problems), provided that it is translation-invariant and that its finite differences on the lattice decay rapidly enough for the far-field multipole expansion on the lattice to be convergent.

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Several "kernel-independent" ("black-box") multipole techniques have already been proposed. In the method due to Ying *et al.* [5], the multipole expansions of the kernel are replaced with a continuous distribution of an equivalent source density on a surface enclosing a given box. This equivalent density is found by matching its potential to the potential of the original sources at a surface in the far field. This approach builds up on the earlier ideas of Anderson [7] and Makino [6]: the use of surface potentials or, alternatively, potentials due to fictitious "pseudoparticles" instead of the multipole expansion. Fong & Darve combined continuous SVD with low-rank approximation of the kernel by Chebyshev polynomials (see [4] and references therein) to produce a FMM. Martinsson [9] uses polyharmonic approximations of the kernel to construct a fast multipole method.

2 The Fast Multipole Method on a Lattice

The fast multipole algorithms (FMA) are usually frequency dependent. If the dimension of the object is above 0.5 wavelengths, MLFMA (Multi-level FMA) works properly, since it uses the dominant propagating wave in the translation process [10]. But if the object size is below 0.1 wavelengths, LFFMA (Low Frequency FMA) is employed [11]. In between, MFFMA (Mixed-form FMA) is used to analytically connect multipole and plane wave expansions [12].

The most important step is that the source-field interaction kernel or the Green's function $G(\mathbf{r}_{ji})$ must be cast into the following translation form:

$$G(\mathbf{r}_{ji}) \quad = \quad \beta^t_{jJ_1}(\mathbf{r}_{jJ_1}) \cdot \bar{\bar{\beta}}_{J_1J_2}(\mathbf{r}_{J_1J_2}) \cdot \bar{\bar{\alpha}}_{J_2I_2}(\mathbf{r}_{J_2I_2}) \cdot \bar{\bar{\beta}}_{I_2I_1}(\mathbf{r}_{I_2I_1}) \cdot \beta_{I_1i}(\mathbf{r}_{I_1i}) \tag{2}$$

where

$$\mathbf{r}_{ji} \quad = \quad \mathbf{r}_{jJ_1} + \mathbf{r}_{J_1J_2} + \mathbf{r}_{J_2I_2} + \mathbf{r}_{I_2I_1} + \mathbf{r}_{I_1i} \tag{3}$$

as plotted in Fig. 1. β_{jJ_1} and β_{I_1i} are column vectors called receiving and radiation patterns, respectively. $\bar{\beta}_{J_1J_2}$ and $\bar{\beta}_{I_2I_1}$ are matrices (dense for low frequencies and diagonal for mid-frequencies) converting incoming and outgoing waves between parent boxes and child boxes. They could be considered as far-field-to-far-field or local-field-to-local-field transformations. $\bar{\alpha}_{J_2I_2}$ is an outgoing-wave to incoming-wave translator (O2I translator), or far-field-to-local-field translator. There are 316 O2I translators for 3D problems. But each time only outgoing waves from nonempty boxes in the interaction list are translated. Mathematically, the addition theorem is used to generate this translation format. Many FMA performance improvements can be realized by working out novel translators.

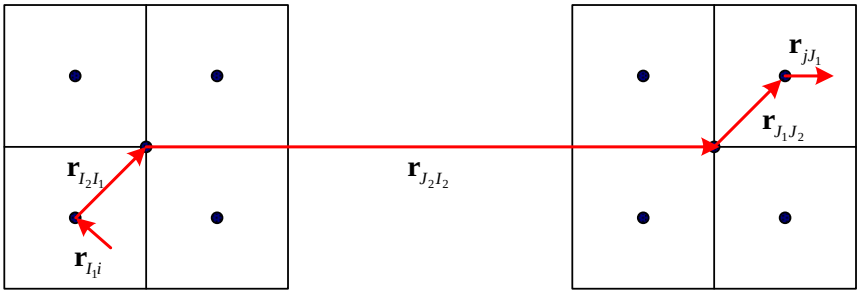

Figure 1: FMA decomposition of the vector $\mathbf{r}_{ji}$. 2D rendition for simplicity.

For the scattering problem, the object size is usually comparable to the wavelength. Hence, MLFMA is employed. The free space Green's function can be decomposed into the integration of plane waves to all directions. From the addition theorem [13], the free space Green's function can be generally represented by

$$\frac{e^{ik|\mathbf{D}+\mathbf{d}|}}{4\pi|\mathbf{D}+\mathbf{d}|} = \frac{ik}{4\pi}\sum_{l=0}^{\infty}(-1)^l(2l+1)j_l(kd)h_l^{(1)}(kD)P_l(\hat{d}\cdot\hat{D}) \tag{4}$$

where $j_l(x)$ is the spherical Bessel function of the first kind, $h_l^{(1)}(x)$ is the spherical Hankel function of the first kind, $P_l(x)$ is the Legendre polynomial, and $d < D$. It is further derived into a diagonal translation format by introducing a plane wave integration, truncating the summation, and exchanging the order of integration and summation

$$\frac{e^{ik|\mathbf{D}+\mathbf{d}|}}{4\pi|\mathbf{D}+\mathbf{d}|} = \frac{ik}{4\pi}\int d\Omega e^{i\mathbf{k}\cdot\mathbf{d}}\alpha_L(\Omega,\mathbf{D}) \tag{5}$$

where $\int d\Omega$ represents the integral over a unit sphere. The far-field-to-local-field translator $\alpha_L(\Omega,\mathbf{D})$ is defined as

$$\alpha_L(\Omega,\mathbf{D}) = \frac{1}{4\pi}\sum_{l=0}^{L}i^l(2l+1)h_l^{(1)}(kD)P_l(\hat{k}\cdot\hat{D}) \tag{6}$$

The term $e^{i\mathbf{k}\cdot\mathbf{d}}$ is a combination of far-field-to-far-field transformations, local-field-to-local-field transformations, radiation patterns and receiving patterns. In the conventional BEM, FMA was applied to sources represented by RWG basis over triangular patches [14].

$$\beta(\hat{k}) = \int_S e^{i\mathbf{k}\cdot\mathbf{r}'}S(\mathbf{r}')dr' \tag{7}$$

On a lattice, the sources are all point sources. Hence, the radiation pattern setup becomes much simpler.

$$\beta(\hat{k}) = \int_S e^{i\mathbf{k}\cdot\mathbf{r}'}\delta(\mathbf{r}')dr' = e^{i\mathbf{k}\cdot\mathbf{r_{Ii}}} \tag{8}$$

Discretization of the integral in (5) results in a diagonal translation form. However, because the Green's function is decomposed into plane waves, essentially we are not using multipoles except for the translator. $\hat{k}$ is sampled over a unit sphere for all angles. The list of $\beta(\hat{k})$ forms the vector of (8).

Because the size of the box doubles when transformations are performed from a lower level of the FMA oct-tree to the parent level, the bandwidth increases correspondingly. Hence, denser data sampling is needed at parent levels. To avoid unnecessary memory at lower levels, interpolation schemes are used during the upward tree browsing process. Hence, (2) is modified by adding the interpolation matrix $\bar{\bar{I}}$

$$G(\mathbf{r}_{ji}) = \beta^t_{jJ_1}(\mathbf{r}_{jJ_1})\cdot\bar{\bar{I}}^t\cdot\bar{\bar{\beta}}_{J_1J_2}(\mathbf{r}_{J_1J_2})\cdot\bar{\bar{\alpha}}_{J_2I_2}(\mathbf{r}_{J_2I_2})\cdot\bar{\bar{\beta}}_{I_2I_1}(\mathbf{r}_{I_2I_1})\cdot\bar{\bar{I}}\cdot\beta_{I_1i}(\mathbf{r}_{I_1i}) \tag{9}$$

The error of this mid-frequency MLFMA is controlled by the truncation number L in the translator and the buffer zone. Because of the computer's limited numerical precision, L cannot be infinitely

large. A lot of work has been done to refine the estimation of L for the best possible accuracy. A very nice estimation is using the following excess bandwidth equation:

$$L \approx kd + 1.8d_0^{2/3}(kd)^{1/3} \tag{10}$$

where $d_0 = \log(1/\epsilon)$. This method is very effective for mid-frequency applications since the accuracy could reach 10^{-5} easily when the box size is large compared to the wavelength. However, when the frequency is low, even the best excess bandwidth equation could not improve the error too much.

The near field interaction is computed directly. The conventional MoM method could be applied to this part to collect the contributions from near neighbors.

3 The Lattice Green Function for the Scalar Wave Equation in 3D

The linear scalar wave equation (the Helmholtz equation) in 3D is

$$\nabla^2 u + k^2 u = f, \tag{11}$$

where k is a given parameter (the wavenumber), f (the source) is a given function of coordinates, and u is an unknown function to be found.

The Green function $G(\mathbf{r})$ for (11) is, by definition, generated by the delta-source $f = \delta(\mathbf{r})$; i.e.

$$\nabla^2 G + k^2 G = \delta(\mathbf{r}), \tag{12}$$

G has the well known analytical form

$$G(\mathbf{r}) = \frac{\exp(\mathrm{i}kr)}{4\pi r} \tag{13}$$

We now consider discrete analogs of (11), (13). Let (12) be approximated by the standard seven-point flux-balance scheme on a uniform grid with a size h (for simplicity, the same in all three directions):

$$(6-k^2h^2)g_{ix+1,iy,iz} - g_{ix-1,iy,iz} - g_{ix,iy+1,iz} - g_{ix,iy-1,iz} - g_{ix,iy,iz+1} - g_{ix,iy,iz-1} = \frac{\delta(ix,iy,iz)}{h} \tag{14}$$

where g is the lattice Green function (LGF), ix, iy, iz are integer indexes, and δ in this expression is the *discrete* delta-function (the Kronecker delta in 3D).

There are at least two general ways to compute the LGF: Fourier analysis and finite difference solutions. A detailed exposition for the Laplace equation has been given by Martinsson & Rodin [9, 8, 15]; for the wave problem, see [17].

Fourier analysis is quite involved and must be performed with great care. For our purposes, a more straightforward route is sufficient. The finite difference problem (14) for the Green function can be solved directly, with the continuous Green function imposed as a boundary condition on a large enough cube $[-M, M]^3$. Such a direct solution can be efficiently obtained via FFT, as done for the Laplace equation by Kansa *et al.* [18].

An example of LGF for $\lambda = 1$ ($k = 2\pi$) and $h = 0.1$ is shown in Fig. 3 (1D plot) and Fig. 3 (surface plot).

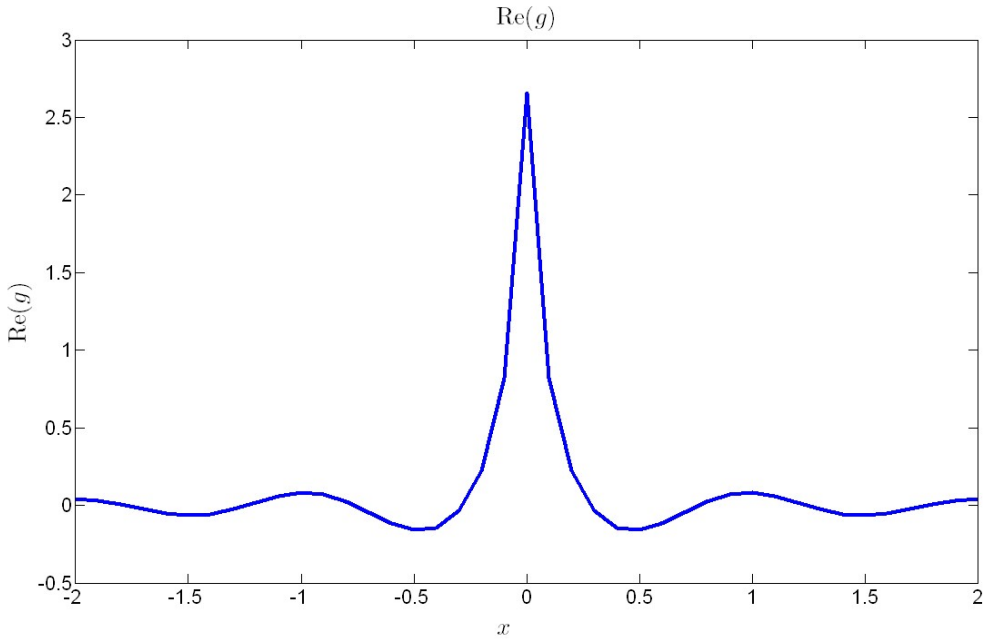

Figure 2: a 1D plot ($y = z = 0$, x varies) of the LGF for $\lambda = 1$, $h = 0.1$.

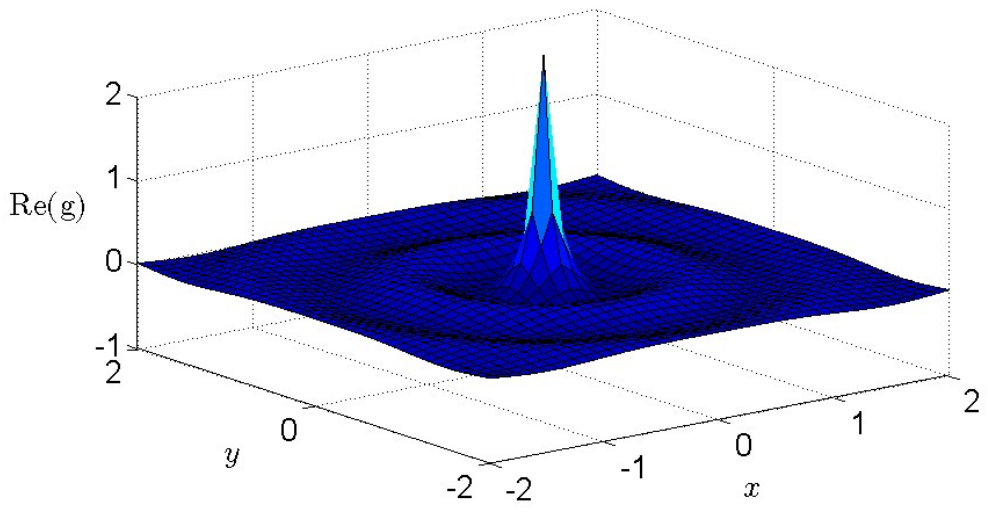

Figure 3: A surface plot ($z = 0$, x, y vary) of the LGF for $\lambda = 1$, $h = 0.1$.

4 Conclusion

The proposed Fast Multipole Method on a lattice has the following salient advantages:

- Close-to-optimal (apart from the logarithmic factors) asymptotic number of operations with respect to the number of grid nodes.
- In applications to finite difference analysis of boundary value problems, the method paves the way for the efficient solution of boundary algebraic equations (Martinsson & Rodin [9, 15]]), or, alternatively, equations of difference potentials – a discrete analog of Calderon projections (Ryaben'kii & Tsynkov [1, 2]). The latter method and its computational efficiency were recently analyzed in detail for problems involving exterior magnetic fields of fusion devices [18].

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